

***Comment on a
Numerical Horizontal Flow Anomaly
with Consideration of the
Second Law of Thermodynamics***

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- > *Insights into “adaptive” modeling*
- > *Horizontal flow anomaly – Part 1*
- > *Entropy balance in open two-phase flow systems*
- > *Irreversible thermodynamics and interface mass and heat transfer*
- > *Entropy generation*
- > *Horizontal flow anomaly – Part 2*
- > *Summary*

Adaptive Modeling. Concept

- > Consider a two-phase flow simulation system, where ...
- > The set of basic equations is extended by irreversible thermodynamic laws and relationships.
- > A positive entropy generation rate is inherently ensured.
- > The *adaption* of existing constitutive relations to this simulation system is called *adaptive modeling*

Adaptive modeling. Interphase mass and heat transfer

- > *Traditional modeling*
(Chow, Ransom, Riemke, Trapp)

Evaporation ($\Gamma_{ig} > 0$)

$$h_g^* = h_{g,sat}$$

$$h_f^* = h_f$$

Condensation ($\Gamma_{ig} < 0$)

$$h_g^* = h_g$$

$$h_f^* = h_{f,sat}$$

- > *Otherwise, it can be shown that the phase change process implies energy transfer from a lower temperature to a higher temperature.*
(RELAP5/MOD2 Manual)

- > *Adaptive modeling*

$$h_g^* = h_{g,sat}$$

$$h_f^* = h_{f,sat}$$

Adaptive Modeling. (Nucleate) Boiling Process

> With given wall heat transfer
(Chen's relation)

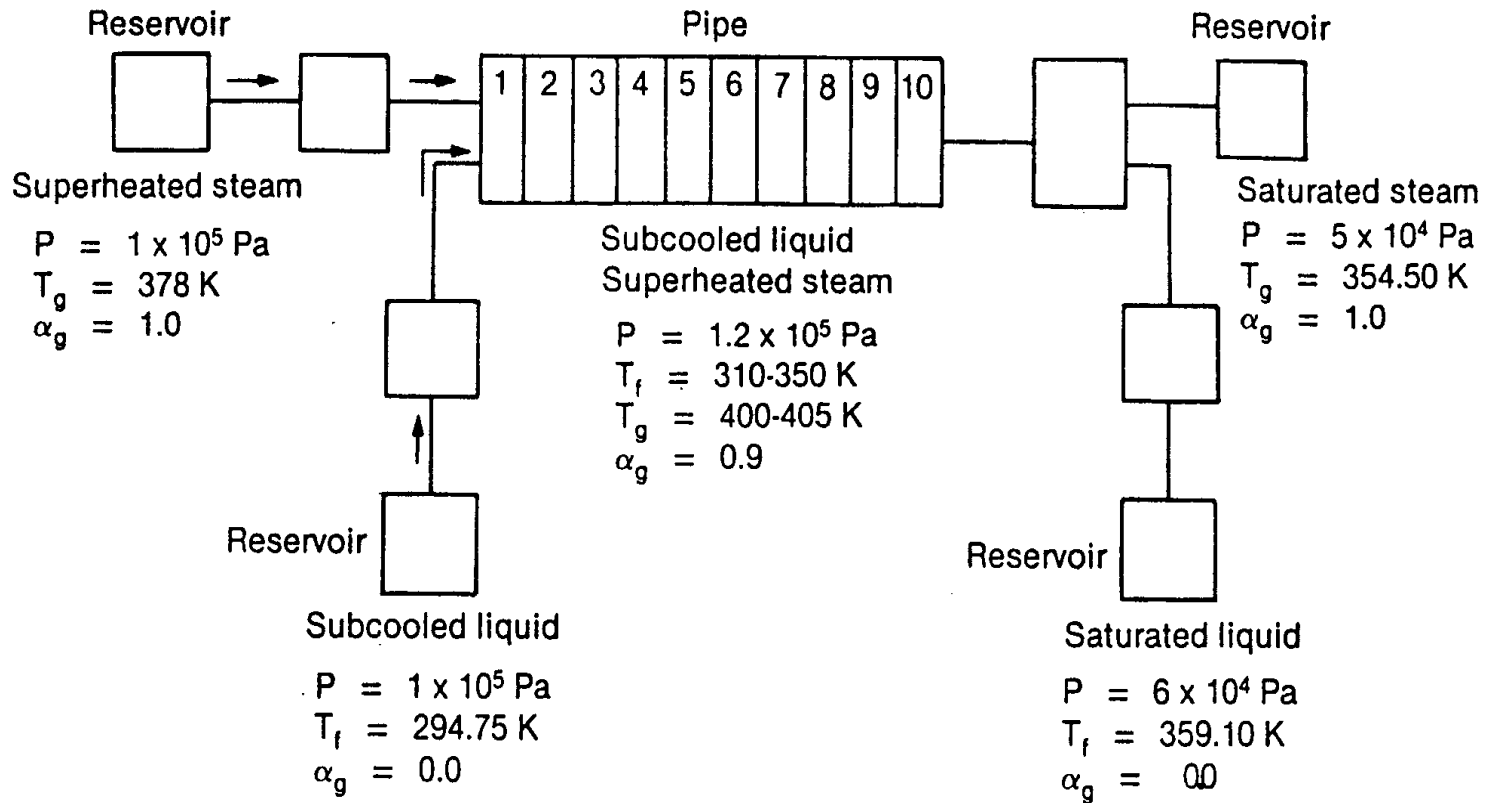
$$q_{\text{Chen}} = -h_{\text{mic}} (T_s - T_f) + 0 \cdot (T_s - T_g) + (h_{\text{mic}} + h_{\text{mac}}) (T_w - T_f)$$

the evaporation rate is determined.

$$\Gamma_w = \frac{A_w}{(h_{g,\text{sat}} - h_{f,\text{sat}}) V} h_{\text{mic}} (T_w - T_f)$$

Horizontal Flow Annular. Experimental Arrangement

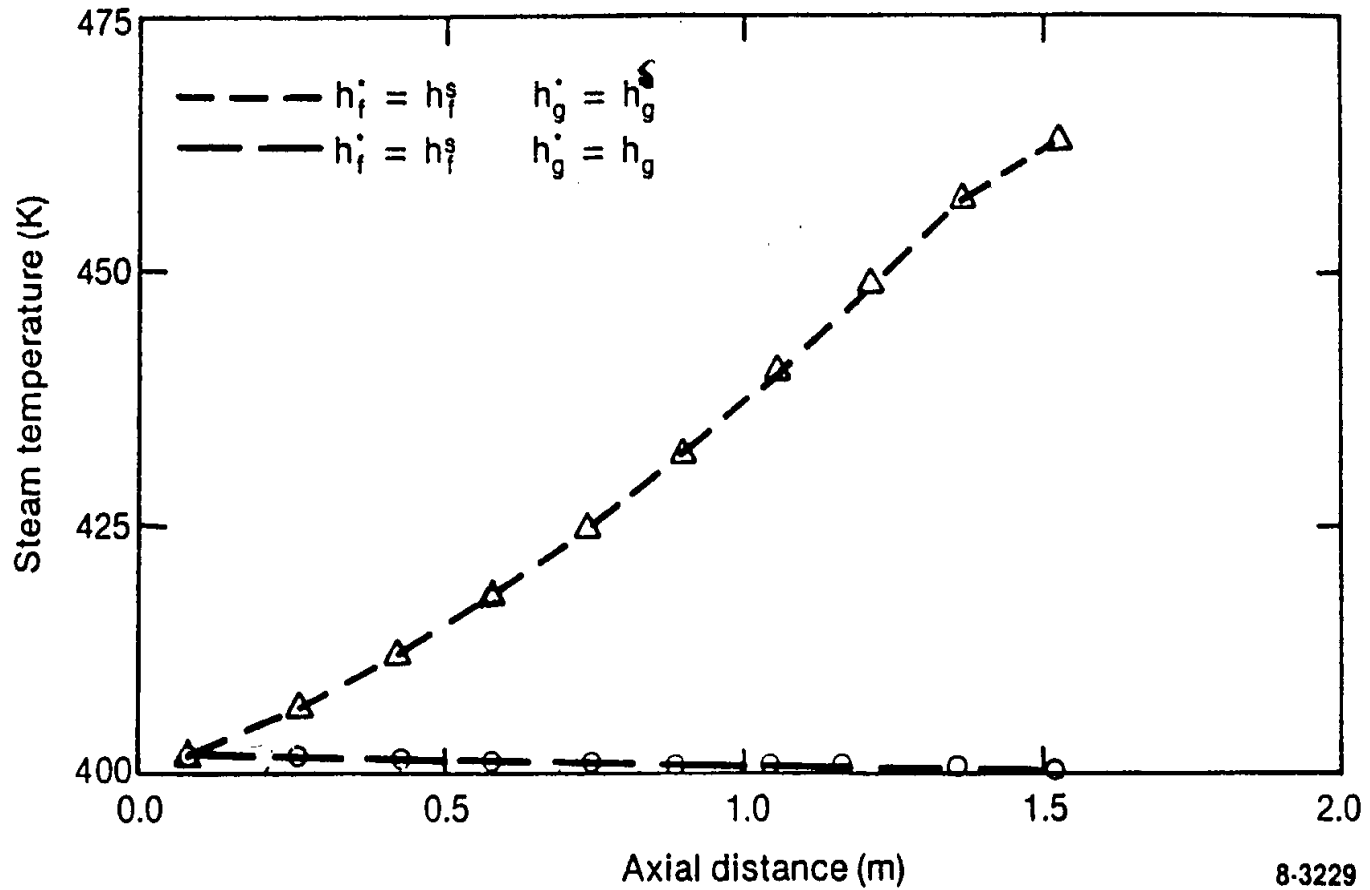
V



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Horizontal flow anomaly. Steam temperature

V



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Entropy balance in open two-phase flow systems (1)

> Energy balance in RELAP5 (liquid phase)

$$\frac{\partial}{\partial t}(\alpha_f \rho_f u_f) + \frac{\partial}{\partial x}(\alpha_f \rho_f u_f v_f) = -p \frac{\partial \alpha_f}{\partial t} - p \frac{\partial (\alpha_f v_f)}{\partial x} + j_2^{u+pv}$$

> Mass balance (liquid phase)

$$\frac{\partial}{\partial t}(\alpha_f \rho_f) + \frac{\partial}{\partial x}(\alpha_f \rho_f v_f) = +j_1^m$$

Entropy balance in open two-phase flow systems (2)

> *Substitution of internal energy*

$$u_f = \mu_f - \frac{p}{\rho_f} + T_f s_f$$

> *Duhem-Gibbs (substitution of derivatives)*

$$du_f = T_f ds_f + \frac{p}{\rho_f} d\rho_f$$

Entropy balance in open two-phase flow systems (3)

> *Entropy balance for the liquid phase*

$$\frac{\partial}{\partial t} (\alpha_f \rho_f s_f) + \frac{\partial}{\partial x} (\alpha_f \rho_f s_f v_f) = -\frac{\mu_f}{T_f} \dot{j}_1^m + \frac{1}{T_f} \dot{j}_2^{u+pv}$$

Entropy balance in open two-phase flow systems (4)

> *Total entropy balance*

$$\begin{aligned}\frac{\dot{S}}{V} &= \frac{\partial}{\partial t} \left(\alpha_f \rho_f s_f + \alpha_g \rho_g s_g \right) + \frac{\partial}{\partial X} \left(\alpha_f \rho_f s_f v_f + \alpha_g \rho_g s_g v_g \right) = \\ &= - \left(\frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) \dot{j}_1^m + \left(\frac{1}{T_f} - \frac{1}{T_g} \right) \dot{j}_2^{u+pv}\end{aligned}$$

> *The entropy source term in RELAP5 is a dot product of fluxes and forces*

Entropy balance in RELAP5 (1)

- > *Interphase mass and heat fluxes in RELAP5 are source terms in the mass and energy balance equations*

$$\dot{j}_1^m = (-\Gamma_{ig}) = \frac{H_{ig}}{h_g^* - h_f^*} (T_{sat} - T_g) + \frac{H_{if}}{h_g^* - h_f^*} (T_{sat} - T_f)$$

$$\dot{j}_2^{u+pv} = \frac{h_f^* H_{ig}}{h_g^* - h_f^*} (T_{sat} - T_g) + \frac{h_g^* H_{if}}{h_g^* - h_f^*} (T_{sat} - T_f)$$

Entropy balance in RELAP5 (2)

> Taylor series expansion of the forces

$$\left(\frac{1}{T_f} - \frac{1}{T_g} \right) = \frac{1}{T_{\text{sat}}^2} \left[(T_s - T_f) - (T_s - T_g) \right]$$

$$-\left(\frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) = \frac{-1}{T_{\text{sat}}^2} \left[h_{f,\text{sat}} (T_s - T_f) - h_{g,\text{sat}} (T_s - T_g) \right]$$

Entropy balance of RELAP5 (3)

$$\begin{aligned}\frac{\dot{S}}{V} &= + \left(\frac{1}{T_f} - \frac{1}{T_g} \right) j^{u+pv} - \left(\frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) j^m = \\ &= + \left[\frac{(h_g^* - h_{f,sat}) H_{if}}{(h_g^* - h_f^*) T_{sat}^2} \right] (T_{sat} - T_f)^2 \\ &\quad - \left[\frac{(h_g^* - h_{g,sat}) H_{if} + (h_{f,sat} - h_f^*) H_{ig}}{(h_g^* - h_f^*) T_{sat}^2} \right] (T_{sat} - T_f)(T_{sat} - T_g) \\ &\quad + \left[\frac{(h_{g,sat} - h_f^*) H_{ig}}{(h_g^* - h_f^*) T_{sat}^2} \right] (T_{sat} - T_g)^2\end{aligned}$$

> *Quadratic form*

> *Verification of the (mathematical) positive-definiteness is non-trivial*

> Fluxes are source terms in the balance equations

$$J_1 = J^m = J_1^m$$

$$J_2 = J^{u+pv} = J_2^{u+pv}$$

> Forces or affinities

$$F_2 = F_u = + \left(\frac{1}{T_f} - \frac{1}{T_g} \right)$$

$$F_1 = F_m = - \left(\frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right)$$

> *Linear dependence of fluxes on forces*

$$\dot{j}^m = \dot{j}_1 = -L_{11} \left(\frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + L_{12} \left(\frac{1}{T_f} - \frac{1}{T_g} \right)$$

$$\dot{j}^{u+pv} = \dot{j}_2 = -L_{21} \left(\frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) + L_{22} \left(\frac{1}{T_f} - \frac{1}{T_g} \right)$$

> *Onsager's law of reciprocity*

$$L_{ik} = L_{ki}$$

> *Comparison of coefficients*

$$\frac{1}{T_{\text{sat}}^2} \left(-L_{11} h_{f,\text{sat}} + L_{12} \right) = \frac{V}{\left(h_{g,\text{sat}} - h_{f,\text{sat}} \right)} H_{\text{if}}$$

$$-\frac{1}{T_{\text{sat}}^2} \left(-L_{11} h_{g,\text{sat}} + L_{12} \right) = \frac{V}{\left(h_{g,\text{sat}} - h_{f,\text{sat}} \right)} H_{\text{ig}}$$

$$\frac{1}{T_{\text{sat}}^2} \left(-L_{12} h_{f,\text{sat}} + L_{22} \right) = \frac{V \cdot h_g^*}{\left(h_{g,\text{sat}} - h_{f,\text{sat}} \right)} H_{\text{if}}$$

$$-\frac{1}{T_{\text{sat}}^2} \left(-L_{12} h_{g,\text{sat}} + L_{22} \right) = \frac{V \cdot h_f^*}{\left(h_{g,\text{sat}} - h_{f,\text{sat}} \right)} H_{\text{ig}}$$

> *Two systems of linear equations to determine L_{12}*

$$L_{12}(\text{mass}) = -\frac{V \cdot T_{\text{sat}}^2 \left(h_{f,\text{sat}} H_{\text{ig}} + h_{g,\text{sat}} H_{\text{if}} \right)}{\left(h_g^* - h_f^* \right) \left(h_{g,\text{sat}} - h_{f,\text{sat}} \right)}$$

$$L_{12}(\text{energy}) = -\frac{V \cdot T_{\text{sat}}^2 \left(h_f^* H_{\text{ig}} + h_g^* H_{\text{if}} \right)}{\left(h_g^* - h_f^* \right) \left(h_{g,\text{sat}} - h_{f,\text{sat}} \right)}$$

> *Therefore:*

$$h_f^* = h_{f,\text{sat}} \quad h_g^* = h_{g,\text{sat}}$$

Irreversible thermodynamics. Entropy generation

> Entropy generation rate is a quadratic form

$$\frac{\dot{S}}{V} = \sum F_i j_i = \sum F_i L_{ik} F_k$$

> Second law of interphase mass and heat transfer

$$L_{11} > 0$$

$$L_{11} \cdot L_{22} - L_{12} \cdot L_{12} > 0$$

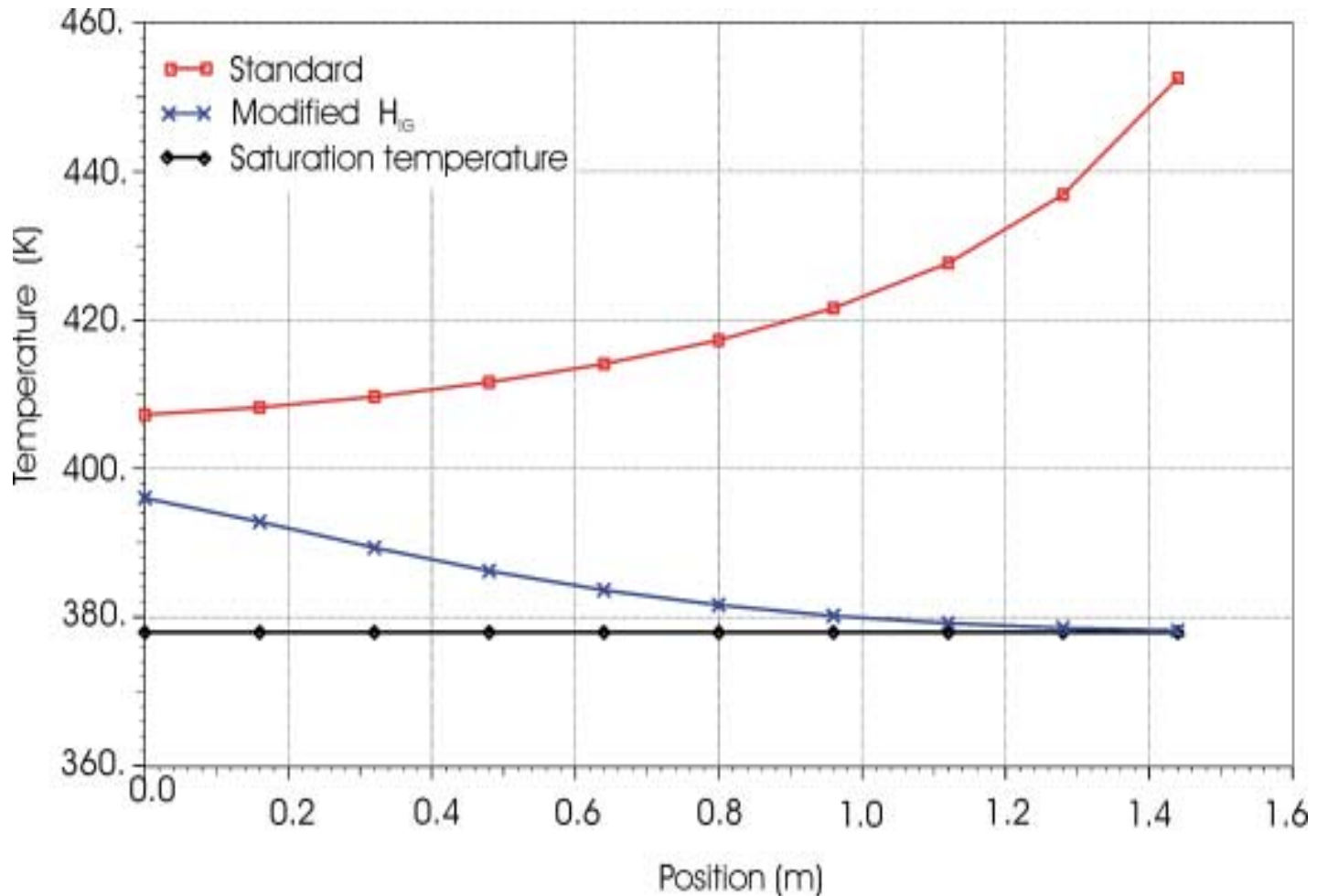
Irreversible Thermodynamics: Entropy generation for interphase mass and heat transfer

$$\begin{aligned}\frac{\dot{S}}{V} &= + \left(\frac{1}{T_f} - \frac{1}{T_g} \right) j^{u+pv} - \left(\frac{\mu_f}{T_f} - \frac{\mu_g}{T_g} \right) j^m = \\ &= + \frac{H_{if}}{T_{sat}^2} (T_{sat} - T_f)^2 + \frac{H_{ig}}{T_{sat}^2} (T_{sat} - T_g)^2\end{aligned}$$

- > *Quadratic form is positive-definite, if H_{if} and H_{ig} are positive*

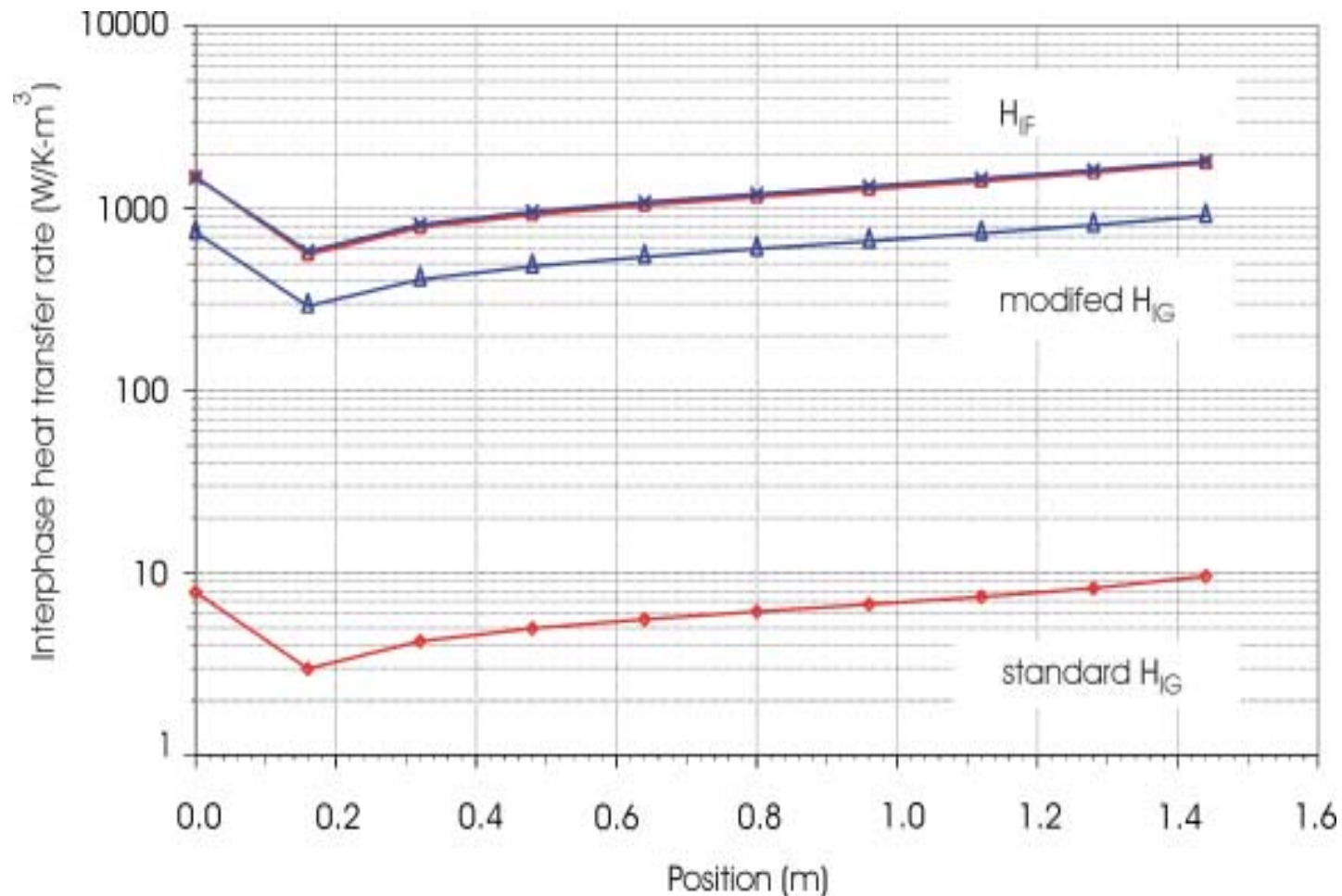
Horizontal flow anomaly. Steam temperatures

> Results



Horizontal flow anomaly. Interphase transfer coefficients

> ... depend on constitutive correlation modeling



- > *The entropy generation rate in RELAP5 can be represented as dot product of fluxes and affinities*
- > *In actual two-phase flow simulation systems the second law is not explicitly considered.*
- > *Irreversible thermodynamics generates a basis for the second law of thermodynamics*
- > *Irreversible thermodynamics describes interphase mass and heat transfer in open flow systems*
- > *The horizontal flow anomaly results from an unphysical choice of constitutive relations*
- > *Finally:*
$$h^* = h_{\text{sat}}$$